

Galaxy(A Web-Based Genome Analysis Tool for Experimentalists) & Pearls(Extract From Past, Prepare For Future)

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1 Galaxy

- 相关背景介绍
- Galaxy简介
- 实例演示
- 参考资料

2 Pearls

- “输入-加工-输出”三段论
- 0-based与1-based
- 基因组版本转换LiftOver
- 基因组数据处理套件EMBOSS
- FASTX-Toolkit
- Excel与TSV的转换
- 文本编辑器
- Unix与Dos的换行符转换
- 用于文本处理的shell指令

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常见的文本操作、解决方案与弊端所在

- 文本操作

显示内容、查看行数;

提取数行/列; 添加删除数行/列;

排序、去冗余;

取交集、并集、补集;

.....



常见的文本操作、解决方案与弊端所在

- 文本操作

- 显示内容、查看行数;

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- 排序、去冗余;

- 取交集、并集、补集;

-

- 解决方案

- 文本编辑器;

- Office (Excel) ;

- 手工处理;

-



常见的文本操作、解决方案与弊端所在

- **文本操作**

- 显示内容、查看行数；
- 提取数行/列；添加删除数行/列；
- 排序、去冗余；
- 取交集、并集、补集；
-

- **解决方案**

- 文本编辑器；
- Office (Excel) ；
- 手工处理；
-

- **弊端所在**

- 大文件打开慢、打不开；
- Excel最多65536行、256列（2007版：1048576行、16384列）
- 手工处理费时费力；
-



- **TSV & CSV**
TSV(Tabular): Tab Separated Values
CSV: Comma Separated Values



- **TSV & CSV**
TSV(Tabular): Tab Separated Values
CSV: Comma Separated Values
- **FASTA, BED, GFF, FASTQ, ...**



- **TSV & CSV**

TSV(Tabular): Tab Separated Values

CSV: Comma Separated Values

- **FASTA, BED, GFF, FASTQ, ...**

- **Interval**

Separator: Tab

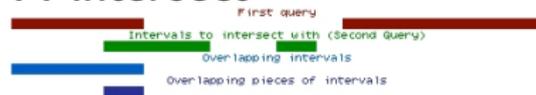
Necessary: Chromosome, Start, End

Optional: Name, Strand, ...

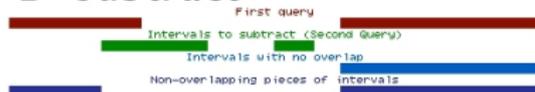


Interval Operations in Galaxy

A Intersect



B Subtract



E Complement



C Merge



D Concatenate



F Cluster



Input

Query 1:					
chr1	10	100	Query1..1		
chr1	500	1000	Query1..2		
chr1	1100	1250	Query1..3		
Query 2:					
				chr1	20
				chr1	2000
				chr1	2500
					80
					2204
					3000
					Query2..1
					Query2..2
					Query2..3

Output

(Return only records that are joined)						Return only records that are joined (INNER JOIN) Return all records of first query (fill null with ".") Return all records of second query (fill null with ".") Return all records of both queries (fill nulls with ".")	
chr1	10	100	Query1..1	chr1	20	80	Query2..1
(Return all records of first query)						Return only records that are joined (INNER JOIN) Return all records of first query (fill null with ".") Return all records of second query (fill null with ".") Return all records of both queries (fill nulls with ".")	
chr1	10	100	Query1..1	chr1	20	80	Query2..1
chr1	500	1000	Query1..2
chr1	1100	1250	Query1..3
(Return all records of second query)						Return only records that are joined (INNER JOIN) Return all records of first query (fill null with ".") Return all records of second query (fill null with ".") Return all records of both queries (fill nulls with ".")	
chr1	10	100	Query1..1	chr1	20	80	Query2..1
.	.	.	.	chr1	2000	2204	Query2..2
.	.	.	.	chr1	500	3000	Query2..3
(Return all records of both queries)						Return only records that are joined (INNER JOIN) Return all records of first query (fill null with ".") Return all records of second query (fill null with ".") Return all records of both queries (fill nulls with ".")	
chr1	10	100	Query1..1	chr1	20	80	Query2..1
chr1	500	1000	Query1..2
chr1	1100	1250	Query1..3
.	.	.	.	chr1	2000	2200	Query2..2
.	.	.	.	chr1	2500	3000	Query2..3



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Galaxy界面(localhost)

The screenshot shows a web browser window titled "Galaxy-Namoroka" with the address bar set to "http://localhost:8080/". The browser's toolbar includes various icons for navigation and search. The Galaxy interface itself has a dark header with the name "Galaxy" and navigation tabs for "Analyze Data", "Workflow", "Shared Data", "Help", and "User".

On the left side, there is a "Tools" panel with a scrollable list of categories such as "Get Data", "Text Manipulation", "Filter and Sort", "Join, Subtract and Group", "Convert Formats", "Extract Features", "Fetch Sequences", "Fetch Alignments", "Get Genomic Scores", "Operate on Genomic Intervals", "Statistics", "Wavelet Analysis", "Graph / Display Data", "Regional Variation", "Multiple regression", "Multivariate Analysis", "Evolution", "Metagenomic analyses", "FASTA manipulation", "NGS: QC and manipulation", "NGS: Mapping", "NGS: Indel Analysis", "NGS: Expression Analysis", "NGS: SAM Tools", and "NGS: Peak Calling".

The main content area features a green banner with a checkmark icon and the text "Hello world! It's running...". Below this is a message: "To customize this page edit static/welcome.html". The central part of the page displays a workflow diagram titled "WWFSMD?" with the subtitle "grow noody appendages...". The diagram consists of several interconnected boxes representing tools, with arrows indicating the flow of data. Below the diagram is the text "usegalaxy.org".

At the bottom of the main content area, there is a line of text: "This project is supported in part by NSF, NHGRI, and the Huck Institutes of the Life Sciences." On the right side of the interface, there is a "History" panel with a message: "Your history is empty. Click 'Get Data' on the left pane to start".

The browser's status bar at the bottom shows search results for "Multiz" and various system icons, including a clock showing "现在: 25 °C" and "今天: 25 °C".



Galaxy 界面(web)

Galaxy-Namoroka

文件(F) 编辑(E) 查看(V) 历史(S) ScrapBook GMarks Ubuntu-It 工具(T) 帮助(H)

http://main.g2.bx.psu.edu/

Galaxy

Galaxy Analyze Data Workflow Shared Data Visualization Help User

Tools Options

- Get Data
- Send Data
- ENCODE Tools
- Lift-Over
- Text Manipulation
- Convert Formats
- FASTA manipulation
- Filter and Sort
- Join, Subtract and Group
- Extract Features
- Fetch Sequences
- Fetch Alignments
- Get Genomic Scores
- Operate on Genomic Intervals
- Statistics
- Graph/Display Data
- Regional Variation
- Multiple regression
- Multivariate Analysis
- Evolution
- Metagenomic analyses
- Human Genome Variation
- EMBOSS

NGS TOOLBOX BETA

- NGS: QC and manipulation
- NGS: Mapping
- NGS: SAM Tools
- NGS: Indel Analysis

Here is what's happening...

Running Your Own Understanding how Galaxy works

An in-depth tutorial

Live Quickies

- Illumina mapping: Single Ends
- Illumina mapping: Paired Ends
- Basic fastQ manipulation:
- Advanced fastQ manipulation:
- 454 Mapping: Single End

The Galaxy team is a part of [BX](#) at Penn State.

This project is supported in part by NSF, NHGRI, The Huck Institutes of the Life Sciences, and The Institute for CyberScience at Penn State.

History Options

Unnamed history

- 5: Subtract on data 4 and data 3
- 16 regions, format: interval, database: hg18
- Info:
- display at UCSC [main](#) | view in [GenSTrack](#) | display at [Ensembl](#) [May 2009](#)
- 1. Chrom 2. Start 3. End 4
- chr01 78762705 78774545 7876
- chr01 103180160 103197643 1031
- chr01 188970651 188981294 1889
- chr01 214554165 214579982 2145
- chr02 141970538 141971752 1419
- chr02 141973472 141980012 1419
- 4: Remove beginning on data 2
- 3: Remove beginning on data 1
- 2: ge_wt.txt
- 1: ge_sample.txt

查找: Multiz

上一个(P) 下一个(N) 全部高亮显示(A) 区分大小写(C) 到达页尾, 从页首继续

图片: 23/23 大小: 107 KB 速度: 6.15 KB/秒 时间: 17.394 一个活动下载项 (剩余 4 小时, 41 分钟) zotero

现在: 25 °C 今天: 25 °C

Four regions

- 1 Masthead: at the top



Four regions

- 1 Masthead: at the top
- 2 Tool menu: on the left-hand side



Four regions

- 1 Masthead: at the top
- 2 Tool menu: on the left-hand side
- 3 **Work area: in the middle**



Four regions

- 1 Masthead: at the top
- 2 Tool menu: on the left-hand side
- 3 Work area: in the middle
- 4 **History panel: on the right**



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Three colours

- **Green background:** a completed query



Four regions

- 1 Masthead: at the top
- 2 Tool menu: on the left-hand side
- 3 Work area: in the middle
- 4 History panel: on the right

Three colours

- **Green background:** a completed query
- **Yellow background with rotating hourglass:** a running query



Four regions & Three colours

Four regions

- 1 Masthead: at the top
- 2 Tool menu: on the left-hand side
- 3 Work area: in the middle
- 4 History panel: on the right

Three colours

- **Green background**: a completed query
- **Yellow background with rotating hourglass**: a running query
- **Gray background with clock icon**: a query in the queue



Several icons

-  shows entire dataset in the browser window



Several icons

-  shows entire dataset in the browser window
-  open metadata editor



Several icons

-  shows entire dataset in the browser window
-  open metadata editor
-  delete item from the history



Several icons

-  shows entire dataset in the browser window
-  open metadata editor
-  delete item from the history
-  **save dataset to the desktop of your computer**



Several icons

-  shows entire dataset in the browser window
-  open metadata editor
-  delete item from the history
-  save dataset to the desktop of your computer
-  refresh OR run the job again



Several icons

-  shows entire dataset in the browser window
-  open metadata editor
-  delete item from the history
-  save dataset to the desktop of your computer
-  refresh OR run the job again
-  **edit history OR dataset tags**



Several icons

-  shows entire dataset in the browser window
-  open metadata editor
-  delete item from the history
-  save dataset to the desktop of your computer
-  refresh OR run the job again
-  edit history OR dataset tags
-  **edit history OR dataset annotation**



Several icons

-  shows entire dataset in the browser window
-  open metadata editor
-  delete item from the history
-  save dataset to the desktop of your computer
-  refresh OR run the job again
-  edit history OR dataset tags
-  edit history OR dataset annotation
-  **collapse all datasets in the history**



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Finding exons with the highest number of SNPs

- 1 Input: exons, snps; UCSC Table Browser



Finding exons with the highest number of SNPs

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- 2 Join[Genomic Operations Join]: identify those exons that contain SNPs



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- 2 Join[**Genomic Operations Join**]: identify those exons that contain SNPs
- 3 **Group: obtain the number of SNPs within each exon**



Finding exons with the highest number of SNPs

- 1 Input: exons, snps; UCSC Table Browser
- 2 Join[**Genomic Operations Join**]: identify those exons that contain SNPs
- 3 Group: obtain the number of SNPs within each exon
- 4 **Sort: sort exon by SNP count**



Finding exons with the highest number of SNPs

- 1 Input: exons, snps; UCSC Table Browser
- 2 Join[**Genomic Operations Join**]: identify those exons that contain SNPs
- 3 Group: obtain the number of SNPs within each exon
- 4 Sort: sort exon by SNP count
- 5 **Filter: filter exons that have ten or more SNPs**



Finding exons with the highest number of SNPs

- 1 Input: exons, snps; UCSC Table Browser
- 2 Join[**Genomic Operations Join**]: identify those exons that contain SNPs
- 3 Group: obtain the number of SNPs within each exon
- 4 Sort: sort exon by SNP count
- 5 Filter: filter exons that have ten or more SNPs
- 6 Join[**Join two Queries**]: restore genomic location for exons containing ten or more SNPs



Finding exons with the highest number of SNPs

- 1 Input: exons, snps; UCSC Table Browser
- 2 Join[**Genomic Operations Join**]: identify those exons that contain SNPs
- 3 Group: obtain the number of SNPs within each exon
- 4 Sort: sort exon by SNP count
- 5 Filter: filter exons that have ten or more SNPs
- 6 Join[**Join two Queries**]: restore genomic location for exons containing ten or more SNPs
- 7 **Visualize: visualize dataset in UCSC Genome Browser**



Share, workflow

- 1 Save: rename the history as “Exons and SNPs”



Share, workflow

- 1 Save: rename the history as “Exons and SNPs”
- 2 Share: share data with others



Share, workflow

- 1 Save: rename the history as “Exons and SNPs”
- 2 Share: share data with others
- 3 **Workflow: generate a workflow from a history in galaxy**



Share, workflow

- 1 Save: rename the history as “Exons and SNPs”
- 2 Share: share data with others
- 3 Workflow: generate a workflow from a history in galaxy
- 4 **Modify: modify a parameter in the workflow in galaxy**



Share, workflow

- 1 Save: rename the history as “Exons and SNPs”
- 2 Share: share data with others
- 3 Workflow: generate a workflow from a history in galaxy
- 4 Modify: modify a parameter in the workflow in galaxy
- 5 Rerun: run workflows with galaxy



Share, workflow

- 1 Save: rename the history as “Exons and SNPs”
- 2 Share: share data with others
- 3 Workflow: generate a workflow from a history in galaxy
- 4 Modify: modify a parameter in the workflow in galaxy
- 5 Rerun: run workflows with galaxy
- 6 **Share: share workflows with galaxy**



Share, workflow

- 1 Save: rename the history as “Exons and SNPs”
- 2 Share: share data with others
- 3 Workflow: generate a workflow from a history in galaxy
- 4 Modify: modify a parameter in the workflow in galaxy
- 5 Rerun: run workflows with galaxy
- 6 Share: share workflows with galaxy
- 7 **Create: generate workflows from scratch with galaxy**
Find the 50 longest exons



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- 1 Home: <http://galaxy.psu.edu/>.
- 2 Wiki: <http://bitbucket.org/galaxy/galaxy-central/wiki/Home>.
- 3 Screencasts: <http://main.g2.bx.psu.edu/screencast>.
- 4 Main: <http://main.g2.bx.psu.edu/>.
- 5 Test: <http://test.g2.bx.psu.edu/>.
- 6 Giardine B, Riemer C, Hardison RC, et al. Galaxy: a platform for interactive large-scale genome analysis. *Genome research*. 2005;15(10):1451-5.
- 7 Taylor J, Schenck I, Blankenberg D, Nekrutenko A. Using galaxy to perform large-scale interactive data analyses. *Current protocols in bioinformatics*. 2007;Chapter 10:Unit 10.5.
- 8 Goecks J, Nekrutenko A, Taylor J, Galaxy Team T. Galaxy: a comprehensive approach for supporting accessible, reproducible, and transparent computational research in the life sciences. *Genome Biology*.
- 9 Blankenberg D, Gordon A, Von Kuster G, et al. Manipulation of FASTQ data with Galaxy. *Bioinformatics (Oxford, England)*. 2010;26(14):1783-5.
- 10 Blankenberg D, Von Kuster G, Coraor N, et al. Galaxy: a web-based genome analysis tool for experimentalists. *Current protocols in molecular biology*. 2010;Chapter 19(January):Unit 19.10.1-21.



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最初输入

数个文件
原始格式
数据缺失

...



三段论

最初输入

数个文件
原始格式
数据缺失

...

中间处理

过滤筛选
添加删除
信息统计

...



三段论

最初输入

数个文件
原始格式
数据缺失
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中间处理

过滤筛选
添加删除
信息统计
...

最终输出

数个文件
规范格式
表格图片
...



最初输入

数个文件
原始格式
数据缺失
...

中间处理

过滤筛选
添加删除
信息统计
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最终输出

数个文件
规范格式
表格图片
...

Three steps all need a key file: **README**

- 1 输入数据：数据来源、格式说明、行列解释、目的要求



最初输入

数个文件
原始格式
数据缺失
...

中间处理

过滤筛选
添加删除
信息统计
...

最终输出

数个文件
规范格式
表格图片
...

Three steps all need a key file: **README**

- 1 输入数据: 数据来源、格式说明、行列解释、目的要求
- 2 处理过程: 程序来源、操作步骤、参数设定、细节解释



最初输入

数个文件
原始格式
数据缺失
...

中间处理

过滤筛选
添加删除
信息统计
...

最终输出

数个文件
规范格式
表格图片
...

Three steps all need a key file: **README**

- 1 输入数据: 数据来源、格式说明、行列解释、目的要求
- 2 处理过程: 程序来源、操作步骤、参数设定、细节解释
- 3 输出文件: 格式说明、行列注解、版本控制、缩写解释



- 文本文件格式: TSV



- 文本文件格式: TSV
- 嵌入注释信息: 位于文件顶端, 以#开头



- 文本文件格式: **TSV**
- 嵌入注释信息: 位于文件顶端, 以#开头
- 列名命名规范: 若干有意义的单词, 首字母大写、单词间无空格, 如: **GeneName**



- 文本文件格式: **TSV**
- 嵌入注释信息: 位于文件顶端, 以#开头
- 列名命名规范: 若干有意义的单词, 首字母大写、单词间无空格, 如: **GeneName**
- 文本文件命名: 以_分隔若干有意义的单词, 并附加年月日, 后缀可有可无 (若有, 一般为txt), 如: **dbSNP130_hg18_UCSC_table_20101001.txt**



- 文本文件格式: **TSV**
- 嵌入注释信息: 位于文件顶端, 以#开头
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- 撰写**README**文件: 清晰、全面、详细



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- 撰写**README**文件: 清晰、全面、详细
- **输入输出文件: 避免程序无法处理的标注, 可以添加一列信息进行替代**



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① Sequence:

0-based index	0	1	2	3	4	5	6	7
sequence	A	A	T	T	G	G	C	C
1-based index	1	2	3	4	5	6	7	8



1 Sequence:

0-based index	0	1	2	3	4	5	6	7
sequence	A	A	T	T	G	G	C	C
1-based index	1	2	3	4	5	6	7	8

2 Coordinates of TT:



0-based & 1-based

1 Sequence:

0-based index	0	1	2	3	4	5	6	7
sequence	A	A	T	T	G	G	C	C
1-based index	1	2	3	4	5	6	7	8

2 Coordinates of TT:

- 0-based, half-open:



0-based & 1-based

1 Sequence:

0-based index	0	1	2	3	4	5	6	7
sequence	A	A	T	T	G	G	C	C
1-based index	1	2	3	4	5	6	7	8

2 Coordinates of TT:

- 0-based, half-open:



1 Sequence:

0-based index	0	1	2	3	4	5	6	7
sequence	A	A	T	T	G	G	C	C
1-based index	1	2	3	4	5	6	7	8

2 Coordinates of TT:

- 0-based, half-open: [2,4)
also known as: 0-based start, 1-based end



1 Sequence:

0-based index	0	1	2	3	4	5	6	7
sequence	A	A	T	T	G	G	C	C
1-based index	1	2	3	4	5	6	7	8

2 Coordinates of TT:

- 0-based, half-open: [2,4)
also known as: 0-based start, 1-based end
- 1-based, fully-closed:



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- **Genome Browser: 1-based, fully-closed:**



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- **Table Browser: 0-based, half-open**



0-based & 1-based

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3 Example:

- Genome Browser: 1-based, fully-closed:
- Table Browser: 0-based, half-open
- **dbSNP: 0-based, half-open**



1 Galaxy

- 相关背景介绍
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2 Pearls

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1 Galaxy

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- **Web interfaces:** <http://emboss.sourceforge.net/interfaces/#web>



1 Galaxy

- 相关背景介绍
- Galaxy简介
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2 Pearls

- “输入-加工-输出”三段论
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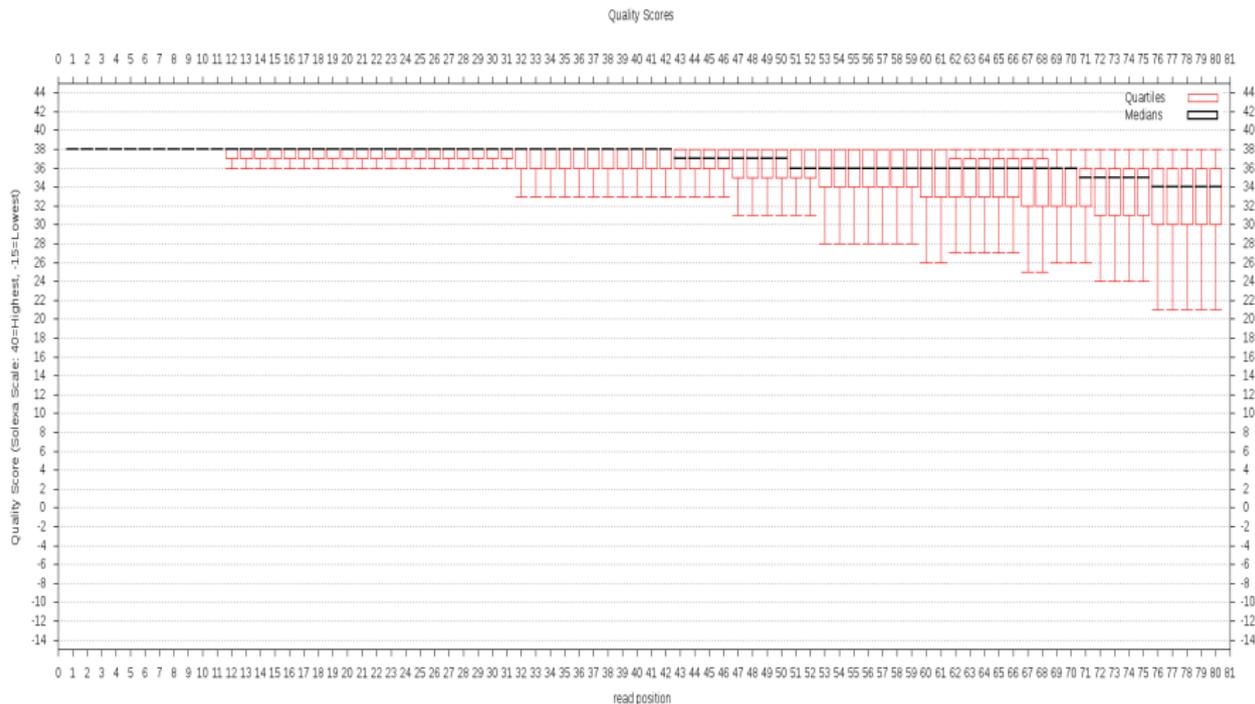
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- Website

http://hannonlab.cshl.edu/fastx_toolkit/





1 Galaxy

- 相关背景介绍
- Galaxy简介
- 实例演示
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2 Pearls

- “输入-加工-输出”三段论
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- Excel \Rightarrow TSV



- Excel ⇒ TSV

- MS office, WPS: 使用另存为功能, 保存类型选择文本文件(制表符分隔)。



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● TSV ⇒ Excel

选择使用Excel打开即可；之后可以另存为xls格式。



1 Galaxy

- 相关背景介绍
- Galaxy简介
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2 Pearls

- “输入-加工-输出”三段论
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推荐使用的编辑器

- **Windows**

- Notepad++: <http://notepad-plus-plus.org/>
- UltraEdit[Not FREE]: <http://www.ultraedit.com/>
- SciTE: <http://www.scintilla.org/SciTE.html>

- **Linux**

- gedit: <http://projects.gnome.org/gedit/>
- Vim: <http://www.vim.org/>
- Emacs: <http://www.gnu.org/software/emacs/>



1 Galaxy

- 相关背景介绍
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- 实例演示
- 参考资料

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- 换行符



- 换行符
 - Windows: `\r\n`(回车+换行),文件尾部直接EOF(文件结束标志)



Unix与Dos的换行符

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- Windows: `\r\n`(回车+换行),文件尾部直接EOF(文件结束标志)
- Unix: `\n`(仅有换行),文件最后一行也会增加该字符,然后才是EOF

```
yixf@Yixf-Ubuntu: ~/Desktop 15:07:02 $ file dos_file unix_file
dos_file: ASCII text, with CRLF line terminators
unix_file: ASCII text
yixf@Yixf-Ubuntu: ~/Desktop 15:07:04 $ █
```



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- Windows: 文本编辑器
- Unix:
Package: `tofrodos`
Command: `fromdos & todos`



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用于文本处理的shell指令

① 显示查看

file; cat, tac, **dog**¹, nl; more, less; head, tail

¹ **GREEN**: 需要自己下载安装

² <http://soap.genomics.org.cn/index.html>



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wc; sort, **msort**², uniq; split, cut, paste, colrm; diff, join, merge, comm

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4 使用帮助

man COMMAND, info COMMAND;
COMMAND -h, COMMAND --help

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sort与msort

```
yixf@Yixf-Ubuntu: ~ 15:39:11 $ sort 4sort
chr10 30 50 D -
chr10 40 80 E +
chr1 50 100 B +
chr1 50 200 A -
chr1 50 200 A +
chr2 10 20 b -
chr2 10 20 B -
chrX 100 200 G +
chrX 30 50 F +
chrX 90 150 H -

yixf@Yixf-Ubuntu: ~ 15:39:31 $ msort -k 'm1[4-],n2,n3,f4,5{+ -}' 4sort
chr1 50 100 B +
chr1 50 200 A +
chr1 50 200 A -
chr2 10 20 B -
chr2 10 20 b -
chr10 30 50 D -
chr10 40 80 E +
chrX 30 50 F +
chrX 90 150 H -
chrX 100 200 G +
```



- FTP/网页服务器
- 在线云存储
- 版本控制
- 数据库
- ……



Thanks for your attention!